EXTENSION OF THE TRANSURANUS FUEL PERFORMANCE CODE FOR UNCERTAINTY/SENSITIVITY ANALYSES AND ITS APPLICATION TO DESIGN-BASED ACCIDENTS (DBA)

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ABSTRACT

We give an overview on the current capabilities of the TRANSURANUS code for probabilistic analyses – including an add-on option for time-dependent uncertainty analyses based on Monte-Carlo sampling.
On the example of one LOCA and one RIA test with irradiated fuel, we discuss the uncertainty analysis of the cladding radial and axial deformation under DBA conditions. We apply single as well as multiple input uncertainties including fuel rod design/manufacturing data, boundary conditions, physical properties and key models.
We demonstrate a first sensitivity analysis covering the correlations of the cladding deformation with the boundary conditions of both tests. The variation of the Pearson's correlation coefficients with time is addressed in particular.
Finally we give an outlook for extending the statistical output processor of TRANSURANUS and compare it to the alternative of applying generic statistical software packages.

1. Introduction

The capabilities of the TRANSURANUS fuel performance code [1] for performing probabilistic analyses are being extended and now include an add-on module for time-dependent uncertainty analyses based on Monte-Carlo sampling [2]. In this paper we demonstrate a part of these extensions and draw attention to the peculiarities of the most relevant input and output quantities in fuel rod performance simulations. We show a preliminary application in simulations of experimental design-based accident (DBA) scenarios imposed on irradiated nuclear fuel. One case is related to a loss-of-coolant (LOCA) accident as part of the IAEA FUMAC project ([3], see also [4,5]) and a second case is based on a reactivity-initiated accident (RIA) that was included in the earlier IAEA project FUMEX-III [6].

In the second section of the paper we outline the uncertainty analysis made with the TRANSURANUS code where we have applied single as well as multiple input uncertainties that include fuel rod design/manufacturing data, boundary conditions, physical properties and key models.

The two DBA test cases are briefly described in the third section of the paper. In the fourth and the fifth section we address the results calculated for the LOCA and the RIA test case, respectively. For both cases we focus on the cladding radial and axial deformation as well as on the fuel centre temperatures. A first sensitivity analysis is performed entailing Pearson's correlation coefficients related to the source terms (i.e. linear heat rates), the main boundary conditions (i.e. cladding outer temperatures) and to the material properties of fuel and cladding. Attention is drawn to the variation of the Pearson's correlation coefficients with time.

In the final section we discuss first findings specific for either LOCA or RIA scenarios. We give an outlook on different possibilities for further extensions of the TRANSURANUS postprocessor including an export option for complementary analysis by e.g. standard statistics software.

2. Scope of uncertainty and sensitivity analysis

Initially, the most relevant capabilities for statistical analyses of fuel performance simulations were established in the earlier URANUS code [7]. Applying the Monte-Carlo technique, already the first versions of TRANSURANUS allowed statistical variations of a large number of input quantities to be simulated according to normal (Gaussian) distributions. The corresponding code input options cover the fuel rod geometry at beginning of life, all prescribed time-dependent quantities (e.g. linear heat rate and coolant or cladding outside temperatures) as well as all material properties (e.g. thermal conductivity, creep) that are applied in the code for fuel, cladding and coolant. Later on the capabilities were extended by introducing additional types of input distributions (uniform, log-normal, Cauchy) and by allowing user-defined lower and upper bounds of the input quantities to be set [8].

Currently the built-in Monte-Carlo (MC) sample generator allows more than 70 different input uncertainties to be considered in the TRANSURANUS code. In the present analysis we have run deterministic simulations for the base irradiations that precede the DBA tests and two types of probabilistic simulations for the accident phases:

1) We have applied a single input uncertainty that should be of high physical importance. To this end we have selected the cladding outer surface temperature for the LOCA case (assuming a Gaussian distribution cut at $2\sigma=2\%$) and the linear heat rate for the RIA case (assuming a Gaussian distribution cut at $2\sigma=10\%$).

2) We have in addition applied uncertainties to a large set of input parameters for fuel rod/manufacturing data, boundary conditions, physical properties and key models. We have followed the schemes for LOCA outlined in [3] (24 parameters). For RIA we have applied the input uncertainties initially recommended for tests on fresh fuel in ref. [9] (13 parameters).

In the statistical analyses of types (1) and (2) a total of 1000 and 2500 simulations, respectively, were generated by the MC method. The number of samples is thus considerably larger than that deduced from Wilk's formula [10] when requiring a confidence level higher than 95% for estimating the 5%/95% percentiles of calculated output.

In the course of the ongoing development of the TRANSURANUS statistics postprocessor a test option for estimating the 5%/95% percentiles of all simulated output quantities has been introduced [2]. It reflects the representation of the fuel rod as a stack of axially symmetric slices that vary in initial geometry, composition as well as time-dependent boundary conditions – and thus entails an analysis of the output's dependences on time and axial position.

The current version also allows for a first sensitivity analysis by means of Pearson's or simple correlation coefficients (SCC) of output quantity y related to input quantity x. They are defined as

$$SCC = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

where the index i corresponds to the different simulations made by the MC generator.

3. DBA test cases

The LOCA case considered in the FUMAC project [3] is based on an irradiation experiment at the OECD Halden Reactor with a refabricated segment of 440 mm fuelled height. The segment was modelled as a stack of 20 slices. The fuel was provided by EDF and was pre-irradiated in a commercial PWR to a burn-up of 61 MWd/kgHM.

The RIA case included in the FUMEX-III project [6] stems from the irradiation experiment FK-1 at the Japanese NSRR test reactor using a refabricated segment of 106 mm fuelled height. The segment was modelled as a stack of 5 slices. The fuel was pre-irradiated in a commercial BWR to a burn-up of 45.1 MWd/kgHM. Details can be found in [11,12].

Both LOCA and RIA cases required the application of the TRANSURANUS restart option because the cladding material properties as well as some models (e.g. for cladding oxidation) must be modified for high-temperature conditions. Thus the base irradiation cycles have been simulated as one deterministic run and the MC sample generator has subsequently been applied to the LOCA and RIA transient phases. This approach is justified as both experiments consist of a base irradiation in a power reactor and a subsequent DBA transient performed in a test reactor.

For the two types of DBA, the main input quantities as well as the related time scales are obviously different. While under LOCA conditions the outer cladding temperature can be considered as main boundary condition, any RIA test is dominated by the inserted reactivity that is applied by means of the linear heat rate as a function of time. Figure 1 illustrates the time dependence of these main input quantities at rod mid-height.

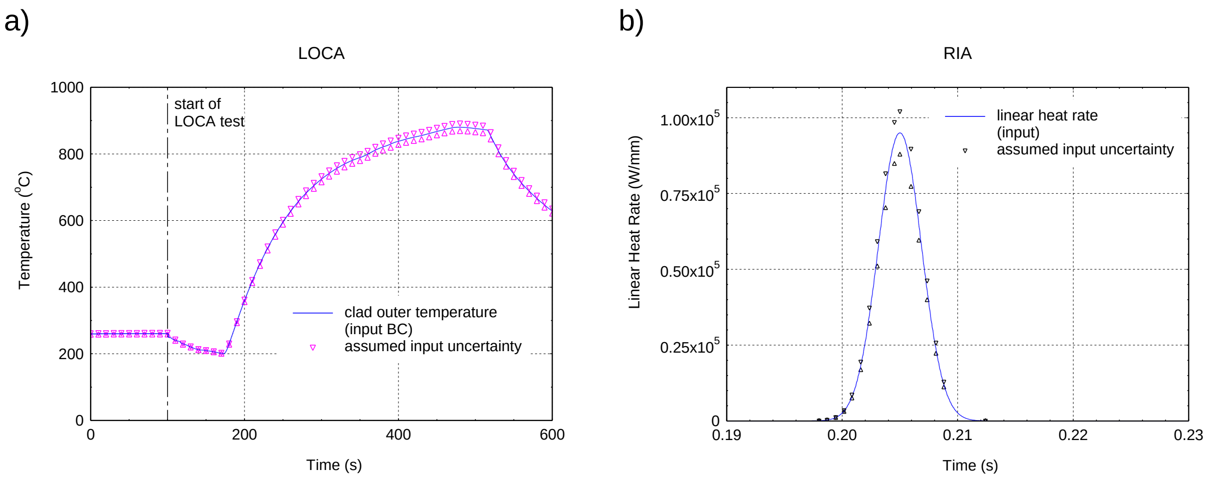

Figure 1: Main input quantities for the two DBA cases analysed in this paper and their applied input uncertainties: a) Outer cladding temperature as main boundary condition in the LOCA case and b) linear heat rate as main source term in the RIA case

4. Simulation of the LOCA test

In this section we discuss the uncertainty analysis of some calculated quantities that are relevant under LOCA conditions: Figures 2a and 3a show the evolution of the cladding radial and axial deformation, respectively. The markers are related to the 5%/95% percentile output uncertainties and the different colours correspond to the analyses of type (1) and (2) as outlined in section 2.

A comparison of the two types of uncertainty analyses illustrates the expected high impact of the cladding outer temperature as the main boundary condition in the LOCA test. Obviously the assumed variation of the clad outer temperature dominates the total output uncertainty band of the cladding outer radius and cladding axial expansion during the 'ballooning' phase up to the simulated time of burst. After this point (t > 367 s) the uncertainty of the given cladding outer temperature still dominates the cladding axial expansion whereas its impact on the cladding outer radius is very small.

The indicated variations with time can be further assessed by a first evaluation of a set of Pearson's or simple correlation coefficients (SCC). They also allow the relative importance of the various inputs to be addressed in more detail (Figures 2b and 3b). We should however note that the correlation coefficients are only computed at the marked points in time and any quantitative conclusions are limited to one specific case.

The uncertainty and sensitivity analysis for the calculated fuel centre temperatures (Figure 4) confirms the significance of the cladding outer temperature as main boundary condition. It increases during ballooning but considerably decreases after burst. While the influence of the linear heat rate on the deformation of cladding is close to zero (cf. Figure 2b and 3b), its impact on the calculated fuel temperatures cannot be neglected (Figure 4b).

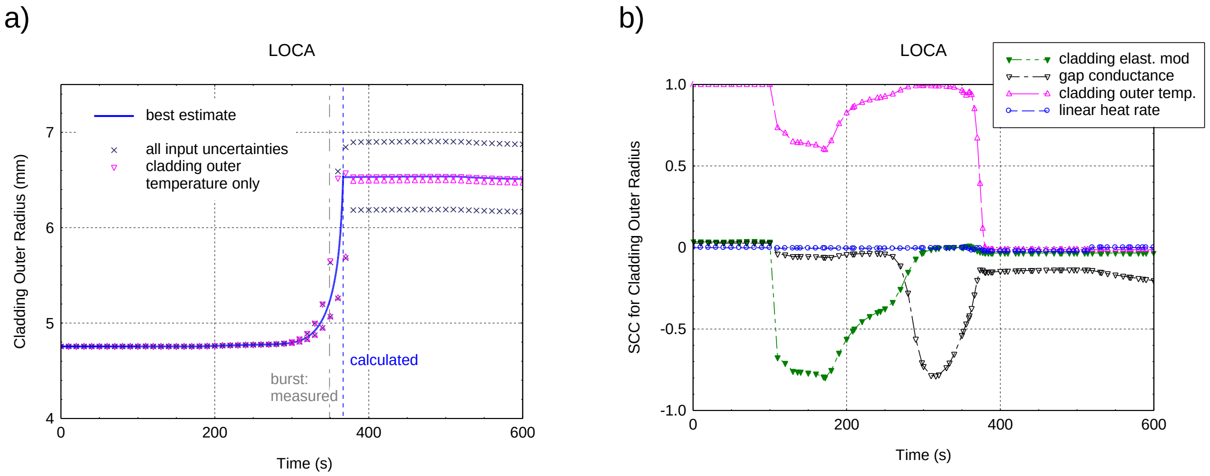

Figure 2: Calculated cladding outer radius at burst node during the LOCA test. a) Uncertainty analysis and b) Pearson's or simple correlation coefficients related to 4 different input quantities. See text for details.

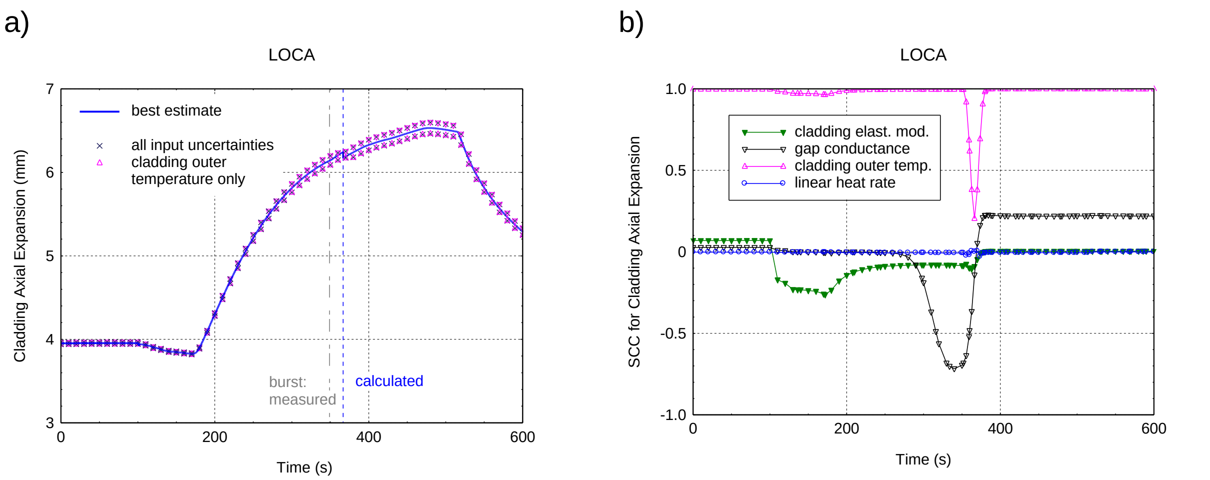

Figure 3: Calculated cladding axial expansion (at the top of the fuel stack) during the LOCA test. a) Uncertainty analysis and b) Pearson's or simple correlation coefficients.

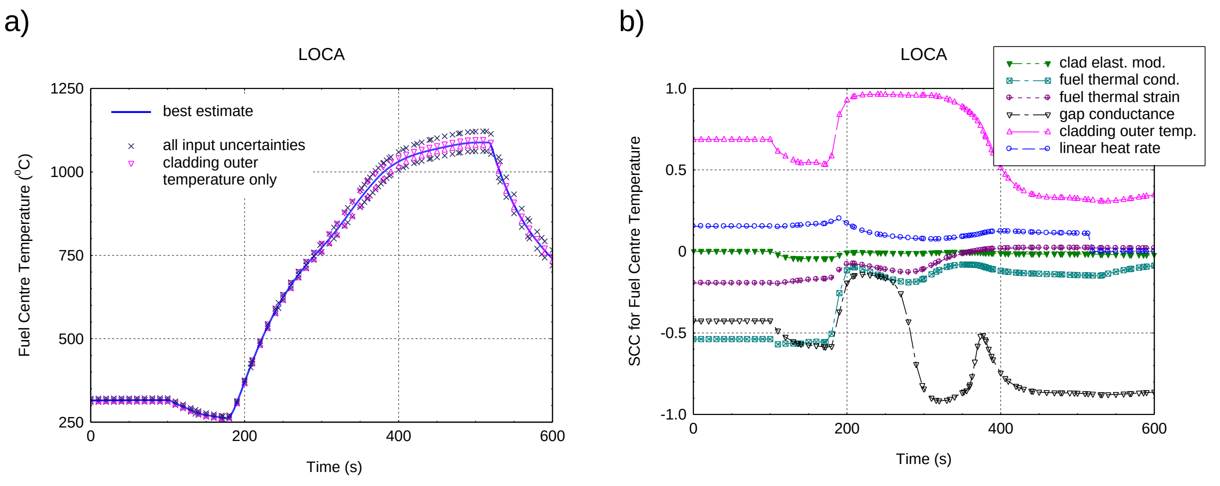

Figure 4: Calculated fuel centre temperatures at burst node during the LOCA test. a) Uncertainty analysis and b) Pearson's or simple correlation coefficients related to 6 different input quantities

For illustration, Figures 2b, 3b and 4b also include the SCC's related to the gap conductance (heat transfer coefficient between fuel and cladding). As expected they show large negative values with an increasing importance during the cladding ballooning phase. The heat transfer coefficient is however not a primary input parameter and any conclusions will require further work. Finally, the present study covers a first evaluation of the SCC's related to some fuel material properties (thermal conductivity and thermal strain). On one hand their impact on the cladding deformation can be neglected, i.e. the SCC's are close to zero and are not shown in Figures 2b and 3b. On the other hand there influence on the simulated fuel temperatures (cf. Figure 4b) is not negligible and should be investigated in more detail.

5. Simulation of the RIA test

Though the physical principles of LOCA and RIA experiments are fundamentally different, the resulting cladding deformation and its dependence on time are of high relevance for both types of tests. Figure 5a shows the evolution of the calculated cladding outer radius for two different phases of the RIA test. The different symbols applied for the 5%/95% uncertainty bands correspond to the two types of input variations (single vs. multiple) as outlined in section 2. For the RIA case we address the single influence of the linear heat rate as the main source term. Both graphs confirm its high impact on the simulated radial deformation of the cladding. For the sake of conciseness the axial expansion of the cladding is not shown because its relative dependence on time as well as the shapes of the uncertainty bands are very similar to those of the radial deformation.

Figure 6 covers the calculated fuel centre temperatures at mid-rod height during the RIA test. The uncertainty bands resulting from the single and multiple input variations are almost equal and underline that the linear heat rate can overshadow second-order effects.

Taking the same approach as for the LOCA test, we have made a first evaluation of a set of Pearson's or simple correlation coefficients (SCC) for the cladding outer radius and for the fuel centre temperatures. They are illustrated in Figures 5b and 6b as follows:

- During the first ('peak') phase of the RIA test we show the SCC's related to the linear heat rate and to the cladding outer temperature.

- During the later phase the two Figures (right side) cover the SCC's related to the heat transfer-coefficient between fuel and cladding (gap conductance) and to the cladding outer temperature.

In any case no quantitative conclusion should be drawn in the current stage of analysis. It is however interesting to note that the SCC's related to the cladding outer temperature reveal a 'change of trend' in the later phase of the RIA (approx. at 2s) that can be linked to the re-opening of the fuel-to-cladding gap (not shown).

Further attention is also needed for interpreting the evolution of the SCC's related to the gap conductance (heat transfer coefficient between fuel and cladding). Both curves (Figure 5b and 6b) indicate a positive correlation in the earlier phase of the RIA test. They change sign in the phase before opening of the fuel-to-cladding gap and show an expected negative correlation under an open-gap condition.

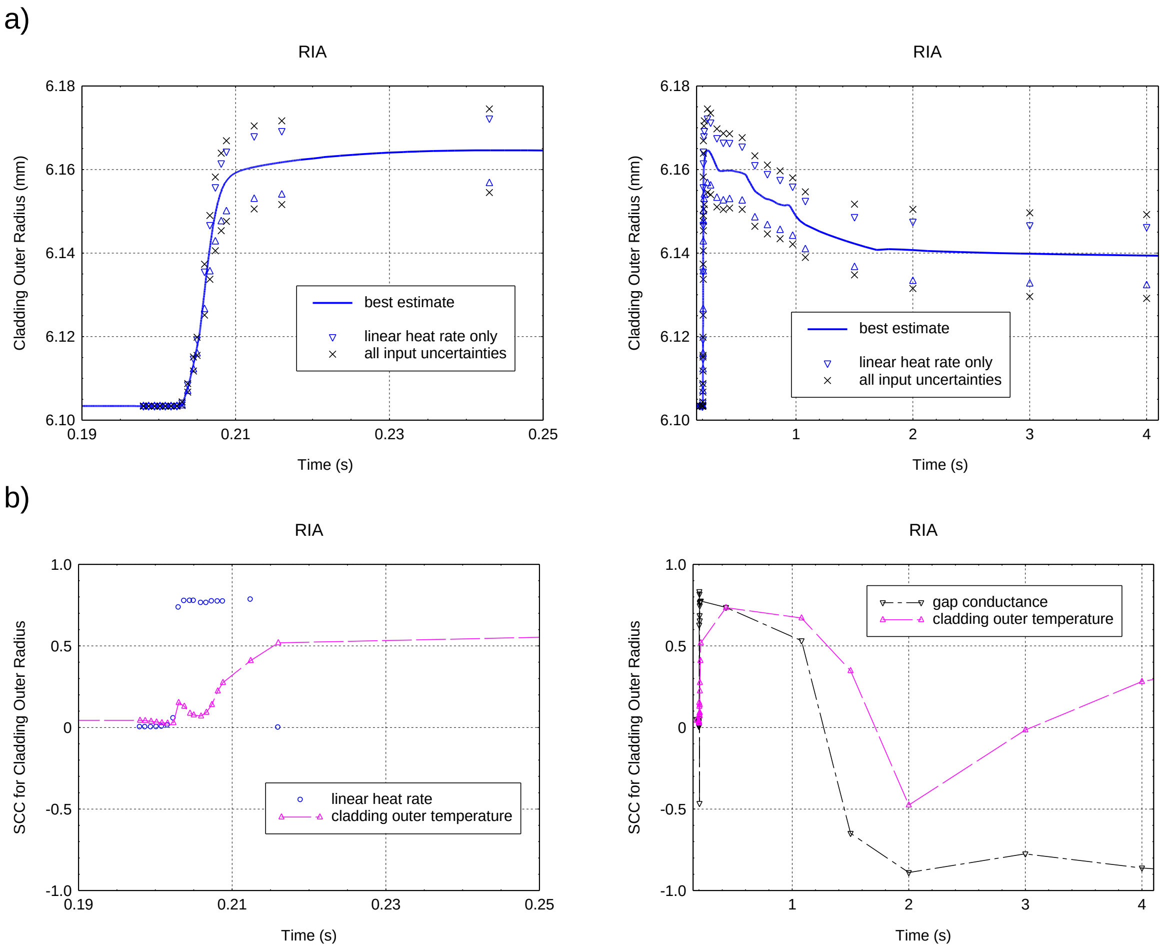

Figure 5: Calculated cladding outer radius at mid-rod height during the RIA test:
a) Uncertainty analysis and b) Pearson's or simple correlation coefficients. See text for details.

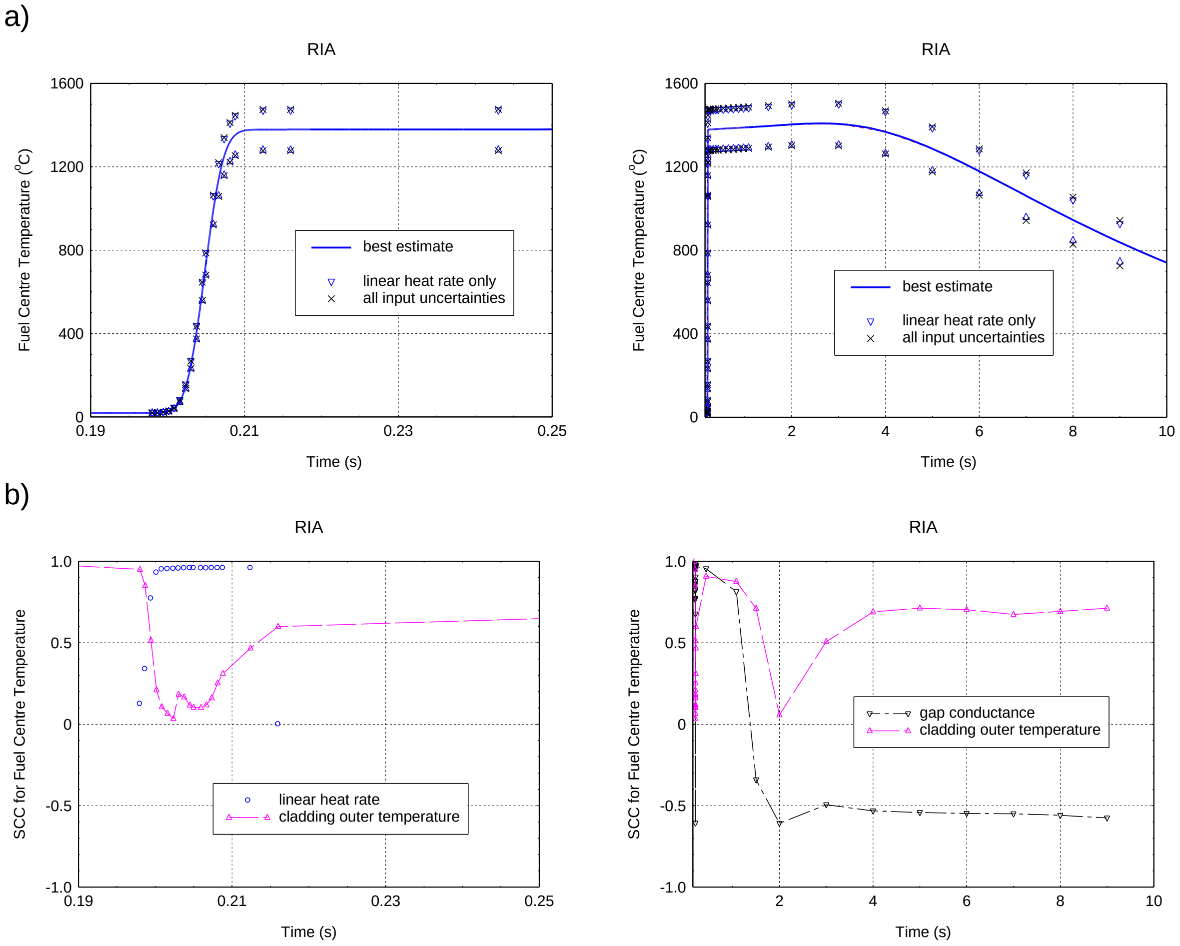

Figure 6: Calculated fuel centre temperatures at mid-rod height during the RIA test:
a) Uncertainty analysis and b) Pearson's or simple correlation coefficients.

6. Summary and outlook

In this paper we have demonstrated some of the capabilities of the TRANSURANUS statistics post-processor that is under development. It includes options for uncertainty and sensitivity analyses and accounts for the peculiarities of time-dependent fuel rod performance simulations.

Depending on future feedback from the user community, we intend to refine the capabilities of the post-processor that should include an interface to more sophisticated statistics analysis software (e.g. DAKOTA [13], SUSY [14], URANIE [15] etc.). Due to the complexity of fuel performance simulations, however, such software requires an appropriate pre-filtering or projection of the output quantities, e.g. in terms of time and axial position. We thus consider setting up an 'export module' in order to complement such functions. In this way a much larger set of estimators and further tools will become available, e.g. the calculation of Spearman correlation coefficients or Sobol's variance decomposition as they had been applied in earlier nuclear fuel behaviour analyses [16,17].

Using a first extension of the TRANSURANUS statistics post-processor we have performed an uncertainty analysis for two DBA scenarios imposed on irradiated nuclear fuel. More precisely, for one LOCA and one RIA case we have estimated the 5%/95% percentiles of the calculated cladding deformation and fuel temperatures. For these output quantities our analysis confirmed the overall dominating impact of the assumed uncertainty of the source terms (i.e. linear heat rates) in the RIA case, and of the main boundary conditions (i.e.

cladding outer temperatures) in the LOCA case. In this context we should draw attention to the potential 'overshadowing' by few input parameters that can be particularly important for transient and for accident conditions.

A preliminary analysis of the Pearson's or simple correlation coefficients (SCC's) underlines the importance of their dependence on time – for both the LOCA and the RIA scenario. The link of the SCC's to different phases of the LOCA and RIA experiment, reflected e.g. by inflection points of fuel temperatures and cladding deformation has been briefly addressed but any detailed physical interpretation requires further work. We also expect that the relative impact of different inputs can vary already under steady-state conditions, e.g. between begin-of-life and end-of-life [18-20]. Such effects should be carefully taken into account before drawing any conclusions on the relative importance of different input uncertainties for safety analyses.

Comprehensive sensitivity analyses are underway in the second phase of the OECD/NEA benchmark for RIA [9,21] and as part of the IAEA FUMAC project for LOCA [3] (using the same case as in this work). So far their findings have been based on maximum or time-averaged correlation coefficients and might have to be complemented by a more detailed time-dependent analysis of the two DBA scenarios. The influence of input uncertainties applied to the base irradiations should be investigated as well. Finally, dependences on the axial and possibly also on the radial position across a fuel rod could be addressed in particular for LOCA conditions.

7. References

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